International Journal of
QUANTUM CHEMISTRY

Contents for Volume 51, 1994, Nos. 1–6 and 52, 1994, Nos. 1–6
Vol. 51, Issue No. 1, 1994

Editorial 1

Properties, Dynamics, and Electronic Structure of Atoms and Molecules

Nonadiabatic NO Expansions for the Ground State Wave Function of H_2^+
G. Blanke and H. Kleindienst 3

Full Configuration Interaction Study of the Ground State of Closed-Shell Cyclic PPP Polyenes
G. L. Bendazzoli, S. Evangelisti, and L. Gagliardi 13

Ab Initio CI Calculations on Benzene with an Extended Basis Set
Y. Yamamoto, T. Noro, and K. Ohno 27

Molecular Structure, Dynamics, and Function of Biological Systems

A Theoretical Investigation of Some Novel Pilocarpine Prodrugs
M. Ekholm and H. Konschin 35

Erratum

Quantum Functional Sensitivity Analysis for the 3-D (J = 0) H + H_2 Reaction
J. Chang and N. J. Brown 53

Diskette Submission Instructions I

Issue No. 2, 1994

Theoretical and Computational Developments

Accurate Computation of Eigenfunctions for Screened Coulomb Potentials
M. A. Núñez 57

Improved Local Density Functional Approach for Atomic Systems
S. K. Ghosh and B. M. Deb 79

Frequency-Dependent Hyperpolarizabilities in the Brueckner Coupled-Cluster Theory
F. Aiga, K. Sasagane, and R. Itoh 87

Properties, Dynamics, and Electronic Structure of Atoms and Molecules

Activation Hardness and Cycloadditions of Even Linear Polyenes
N. K. Ray and R. C. Rastogi 99

Molecular Structure, Dynamics, and Function of Biological Systems

Protonation-Induced Conformational Flipping in Hypermodified Nucleic Acid Base N^6-(*N*-glycylcarbonyl) Adenine
R. Tewari 105

Diskette Submission Instructions I

Issue No. 3, 1994

Theoretical and Computational Developments

Calculating Excitation Energies with the Help of Cumulants
T. Schork and P. Fulde 113

Self-dual Phase-Space Representation of Quantum Mechanics and the Variational Principle
J. J. Włodarz 123

Properties, Dynamics, and Electronic Structure of Atoms and Molecules

The Helium Atom in Its Ground State Embedded in Strong Magnetic Fields
J. F. Rivas-Silva 135

Dimer Form of 1,3-Dimethyluracil Studied by the AM1 Semiempirical Method
M. A. Palafox, N. Iza, and M. Gil 141

A Comparison of Semiempirical and Ab Initio Transition States for HF Elimination in Unimolecular Decompositions
A. J. Mulholland and W. G. Richards 161

Properties, Dynamics, and Electronic Structure of Condensed Systems

The Band Gap of Alternant 1D π-Electron Systems
N. Tyutyulkov, F. Dietz, D. J. Klein, W. A. Seitz, and T. G. Schmalz 173

Diskette Submission Instructions 1

Issue No. 4, 1994

Theoretical and Computational Developments

An Extension of Frost–Musulin and Mobius–Zimmerman Diagrams
Z. Zhou 181

Modified Valence Indices from the Two-Particle Density Matrix
R. F. Nalewajski and J. Mrozek 187

Properties, Dynamics, and Electronic Structure of Atoms and Molecules

A Density-Functional Method for Calculating Atomic Polarizabilities: Application to Negative Ions
M. K. Harbola 201

Accurate Upper and Lower Bounds to the ^2S States of the Lithium Atom
A. Lüchow and H. Kleindienst 211

Ground-State Correlation Energy of Ne
T. Noro, K. Ohtsuki, and F. Sasaki 225

Molecular Structure, Dynamics, and Function of Biological Systems

The Structure of Water in Human *ras* Oncogene Proteins
J. Y. Yu, J. K. Shin, and M. S. Jhon 241

Diskette Submission Instructions I

Issue No. 5, 1994

Theoretical and Computational Developments

Semisimilarity of Molecular Bodies: Scaling–Nesting Similarity Measures
P. G. Mezey 255

Path Integral Approach to Correlation Energy
H. Kawabe, K. Nishikawa, and S. Aono 265

Direct Solution of the Many-Body Schrödinger Equation in the Hyperspherical Formalism: Formulation of the CFHH–GLF Method
W. Bian and C. Deng 285

On Exact Calculation of Response Properties of Oscillators in Static Electric Field: A Fourier Grid Hamiltonian Approach. I. One-Dimensional Systems
P. Dutta and S. P. Bhattacharyya 293

Properties, Dynamics, and Electronic Structure of Atoms and Molecules

Linear Response Calculation of Potential Energy Curves of BH
M. Jaszuński 307

Theoretical Study of Structure and Basicity of Some Alkali Metal Oxides, Hydroxides, and Amides
P. Burk and I. Koppel 313

Properties, Dynamics, and Electronic Structure of Condensed Systems

Incidence of the Muffin-Tin Approximation on the Electronic Structure of Large Clusters Calculated by the MS–LSD Method: The Typical Case of C_{60}
H. Razafinjanahary, R. Rogemond, and H. Chermette 319

Electron Crystallization in Two Dimensions
K. Iyakutti and R. R. Palanichamy 329

Molecular Structure, Dynamics, and Function of Biological Systems

Electrostatic Potential and Electric Field Mapping of Some Sweeteners of the Suosan Series: A Search for the Structure–Activity Relationship
C. Santhosh and P. C. Mishra 335

Diskette Submission Instructions I

Issue No. 6, 1994

Special Issue: Proceedings of the First Congress on Theoretical Chemical Physics. I

Theoretical and Computational Developments

Preface 343

Some Convergence Aspects of the One-Center Expansion Methods
A. Bouferguene and M. Fares 345

Numerical Procedures in Electrochemical Simulation
J. Cecilia, J. Galceran, J. Salvador, J. Puy, and F. Mas 357

Self-Consistent Approximate Solution of the Second-Order Contracted Schrödinger Equation
F. Colmenero and C. Valdemoro 369

Self-Consistent Second-Order Screening in Many-Body Theory
V. E. Van Doren, P. E. Van Camp, and G. Straub 389

Orbitals Expanded in Slater Functions with Single-Exponent by Shell and by Subshell
J. M. Garcia de la Vega and B. Miguel 397

Improvement of Methods for Molecular Dynamics Intergration
D. Janežič and B. Orel 407

Developments in Multicenter Molecular Integrals over STOs Using Expansions in Spherical Harmonics
H. W. Jones 417

Statistical Theory of Spectra
J. Karwowski 425

A New Model of a Molecule Based on the Soft Body
J. Konarski 439

Theory of the Expansion of Wave Functions in a Gaussian Basis
W. Kutzelnigg 447

Thermal Reaction Rates with a Two-Point Flux–Flux Correlation Function
R. Lefebvre, N. Moiseyev, and V. Ryaboy 465

Some Current Problems in Theoretical Chemical Physics to be Solved
P.-O. Löwdin 473

Statistical Properties of Spin-Adapted Reduced Hamiltonians
V. Mas, J. Planelles, J. Karwowski, and R. Rajadell 487

Temporal Rearrangement of Electronic Densities in Slow Atomic Collisions
D. A. Micha 499

A Microscopic Theory for Solution Chemical Reactions: Introduction of Reactant and Medium Structures into Generalized Langevin Equation Formalism
M. Nagaoka, Y. Okuno, N. Yoshida, and T. Yamabe 519

Many-Electron, Many-Photon Theory of Nonstationary States
C. A. Nicolaides, Th. Mercouris, Y. Komninos, and I. D. Petsalakis 529

Mathematical Characterization and Shape Analysis of Localized, Fractal, and Complex Distributions in Extended Systems
J. Pipek and I. Varga 539

Quantum Phase-Space Densities for a Quartic Oscillator
G. G. De Polavieja, F. Borondo, and R. M. Benito 555

Functional Derivative $\delta E/\delta\rho$ in Calculation of Chemical Potential for the Kohn–Sham Electronic System
K. Tkacz-Śmiech, W. S. Ptak, A. Koleżyński, and J. Mrugalski 569

Diskette Submission Instructions I

Vol. 52, Issue No. 1, 1994

Special Issue: Proceedings of the First Congress on Theoretical Chemical Physics. II

Properties, Dynamics, and Electronic Structure of Atoms and Molecules

A Comparative Study on the Structure of M_2Se and M_2I^+ (M = Ag, Au) Using Pseudopotentials and Full Ab Initio Methods
P. Alemany, J. J. Novoa, and L. Bengtsson 1

Vibrational Stark Effect and Vibrational Static Electric Properties of N_2O
J. L. Andrés, J. Bertrán, M. Duran, and J. Marti 9

A Comprehensive Approach to Molecular Charge Density Models: From Distributed Multipoles to Fitted Atomic Charges
J. G. Ángyán and C. Chipot 17

Theoretical Evolution of the Third-Order Molecular Polarizabilities as a Function of Chain Length in Thiophene and Pyrrole Oligomers
D. Beljonne, Z. Shuai, and J. L. Brédas 39

Application of the GCA to a Series of Curve Crossing Topologies
J. Broeckhove, W. Keutgens, L. Lathouwers, and P. van Leuven 49

On the Determination of Effective One-Electron Hamiltonians to be Used for Studying Large Molecules
M. Couty and B. Lévy 59

Dynamics of Photochemical Reactions: Simulation by Quantum Calculations for Transition Metal Hydrides
C. Daniel, M. C. Heitz, L. Lehr, T. Schröder, and B. Warmuth 71

Theoretical Study of the Conjugation Length Effect on the Electronic and Second-Order Nonlinear Optical Properties of Amino–Nitro Diphenylacetylenes
C. Dehu and J. L. Brédas 89

Ab Initio Calculations of Isotropic Hyperfine Coupling Constants in β-Ketoenolyl Radicals
A. Fortunelli 97

MBOHO Calculations of C—H Stretching Frequencies in Hydrocarbons and Heterosubstituted Hydrocarbons
Z.-M. Hu and C.-G. Zhan 109

Ab Initio Calculations to the Reactions of HF and HCl with $Si(OH)_4$ and $(HO)_3SiOSi(OH)_3$: Modeling of SiO_2 Etching Reactions
A. Jenichen 115

Application of Many-Body Perturbation Theory in the Localized Representation for the All-*trans* Conjugated Polyenes
E. Kapuy, F. Bogár, and E. Tfirst 127

Core Photoionization Satellites in Fullerene and Related Model Systems
S. Lunell, C. Enkvist, M. Agback, S. Svensson, and P. A. Brühwiler 135

Iso-Energy Cutoff for the Calculation of Interionic Potential of Mean Force in Water
M. Mezei 147

Nuclear Spin–Spin Coupling and Nuclear Motion
W. T. Raynes, J. Geertsen, and J. Oddershede 153

A Vibrational Hamiltonian Model for Triatomic Molecules Based on the Kratzer and Poschl Teller Potentials
A. Requena, M. Alacid, A. Bastida, and J. Zúñiga 165

Theoretical Study of the Structure and Vibrational Spectra of the $(H_2O)_2 \cdots HF$ and $H_2O \cdots (HF)_2$ Molecular Complexes
C. Rovira, P. Constans, M.-H. Whangbo, and J. J. Novoa 177

Theoretical Investigation of the Enantioselective Hydrogenation of α-Ketoesters over Pt/Alumina Modified with Cinchonidine
O. Schwalm, J. Weber, B. Minder, and A. Baiker 191

Structure and Stability of BN Microclusters: Ab Initio Calculations for $(BN)_n (n = 2–4)$
A. Sutjianto, R. Pandey, and J. M. Recio 199

On the Accuracy of Molecular Properties by Coupled-Cluster Methods for Some Difficult Examples: Oxygen Atom, Iron Atom, and Cyano Radical
M. Urban, J. D. Watts, and R. J. Bartlett 211

Internal Dynamics of Simple Floppy Molecules
L. Zülicke, Ch. Zuhrt, X. Chapuisat, and C. Saint-Espès 227

The Role of the Bond Midpoint Electron Density in Homonuclear Molecular Binding
N. H. March 247

Diskette Submission Instructions I

Issue No. 2, 1994

Special Issue: Proceedings of the First Congress on Theoretical Chemical Physics. III

Properties, Dynamics, and Electronic Structure of Condensed Systems

A Density Functional Elongation Method for the Theoretical Synthesis of Aperiodic Polymers
Y. Aoki, S. Suhai, and A. Imamura 267

Character of the Electronic Ground State and of Charge-Transfer Excited States in Ionic Solids: An Ab Initio Cluster Model Approach
J. Casanovas, A. Lorda, C. Sousa, and F. Illas 281

Quantum Chemical Calculation of Nickel and Copper Atomic Valencies in Crystalline Oxides
R. A. Evarestov, I. I. Tupitsin, and V. A. Veryazov 295

Some Remarks Concerning Spherulitic Growth
A. Gadomski and J. Łuczka 301

Calculations of the Electronic Structure of Various Aperiodic Polymers by an Elongation Method
A. Imamura, Y. Aoki, K. Nishimoto, Y. Kurihara, and A. Nagao 309

Effective Crystal Field Approach to the Binding Energy Calculation of Alkaline Metals
A. Kolezyński, W. S. Ptak, and K. Tkacz-Śmiech 321

Alternating Charge Densities, Peierls Distortion, and Charge-Conjugation Symmetry in Correlated One-Dimensional Diatomic Systems
V. A. Kuprievich 329

Simulation of Diffusion-Limited Aggregation and Reactions Over Its Surfaces
S.-L. Lee and C.-K. Lee 339

Recent Developments in the Theoretical Design of Low-Gap Polymers and Their Nonlinear Optical Properties
P. Otto 353

Electronic Structure and Properties of Hexagonal Wurtzite-type SiC
E. Ruiz, S. Alvarez, and P. Alemany 365

Disordered Grown Systems: Generation and Fractal Analysis. Electrodeposition
F. Sagués, L. López-Tomàs, J. Mach, R. Reigada, P. P. Trigueros, E. Vilaseca, J. Claret, and F. Mas 375

Cooperativity and Electron Correlation Effects on Hydrogen Bonding in Infinite Systems
S. Suhai 395

Electron Correlations and Pairing in Low-Dimensional Systems
I. I. Ukrainskii 413

Statistical Mechanical Theory of Liquid Entropy
D. C. Wallace 425

Molecular Dynamics Simulations of *n*-Alkane Melts Confined Between Solid Surfaces
R. G. Winkler, A. Gerstmair, P. Reineker, T. Matsuda, and D. Y. Yoon 437

Applications to Biological Systems

The Character of the Correlations in DNA Sequences
B. Borštnik 457

Density Functional Studies on Hydrogen-Bonded Complexes
M. Kieninger and S. Suhai 465

Evaluation of Electronic Matrix Elements of Long-Range Electron Transfer in Proteins by the Recursive Residue Generation Method
Y. Mikami 479

Theory of Hopping Conductivity of Proteins
Y.-Y. Ye and J. Ladik 491

Theoretical and Computational Developments

Continuum Wavefunctions by Least-Squares Scheme in a B-Spline Basis: Multicenter and Multielectron Formulations
P. Decleva, M. Brosolo, A. Lisini, and M. Venuti 507

The Onset of Classical Chaos in Atom–Surface Scattering
R. Gauntes, F. Borondo, C. Jaffé, and S. Miret-Artés 515

Properties, Dynamics, and Electronic Structure of Atoms and Molecules

Theoretical Study of Many-Body Effects in the Photoelectron Spectra of Unsaturated Hydrocarbons
A. Lisini, G. Fronzoni, and P. Decleva 527

Calculation of Excitation and Photoionization Spectra by Quasi-Degenerate Perturbation Theory
A. Lisini and P. Decleva 549

The Interaction of Chemical Bonds. III. Perturbed Strictly Localized Geminals in LMO Basis
P. R. Surján 563

Diskette Submission Instructions I

Issue No. 3, 1994

Theoretical and Computational Developments

Analysis of Chemical Phenomena by Solving Constrained Hartree–Fock Equation. I. Method and Application to Resonance Energy in Linear Polyenes
H. Ichikawa and H. Kagawa 575

Computation of Algebraic Formulas for Wigner 3-*j*, 6-*j*, and 9-*j* Symbols by Maple
S.-T. Lai 593

Path Integral's Semiclassical Quantification
J. Marañón 609

Potential-Barrier Model at Metal Surfaces: Thin Films and Its Dependence on the Film Thickness
E. E. Mola, C. A. Paola, and J. L. Vicente 617

Properties, Dynamics, and Electronic Structure of Atoms and Molecules

Semiempirical Quantum Chemical Treatment of the Standard Reduction Potentials of Quinone and Plastoquinone in Water
B. Mallik and S. N. Datta 629

Theoretical Conformational Study of the Stabilities and Geometries of [2, 2] (2, 7) naphthalenophane-1,11-diene and Related Compounds
M^a. J. Rioseras-Garcia and J. M^a. Hernando-Huelmo 651

Electronic Structure and Optical Properties of a Tin-Encapsulated Nickel Porphyrazine Compound
X. L. Liang, D. E. Ellis, O. V. Gubanova, B. M. Hoffman, and R. L. Musselman . 657

Calculations on the Spectra and Nonlinear Third-Order Optical Susceptibility of C_{70}
J. Li, J. Feng, and C. Sun 673

Molecular Structure, Dynamics, and Function of Biological Systems

Comparison of Quantum Mechanical Methods to Compute the Biologically Relevant Reactivities of Cyclopenta-Polycyclic Aromatic Hydrocarbons
J. R. Rabinowitz and S. B. Little 681

Diskette Submission Instructions I

Issue No. 4, 1994

Special Issue on the Applications of Density Functional Theory

Introduction to the 1993 Como Meeting
P. Fantucci and N. Russo 693

Transition States and Energy Barriers from Density Functional Studies: Representative Isomerization Reactions
Y. Abashkin, N. Russo, and M. Toscano 695

An Analysis of the Integrand Occurring in Correlation Energy Functionals
A. Fortunelli and O. Salvetti 705

An Analysis of Nonlocal Density Functionals in Chemical Bonding
R. van Leeuwen and E. J. Baerends 711

The Determination of Intrinsic Reaction Coordinates by Density Functional Theory
L. Deng and T. Ziegler 731

A Mass Formula for the Energy of Metal Clusters
A. Mañanes, M. Membrado, A. F. Pacheco, J. Sañudo, and L. C. Balbás 767

Numerical Grids For Density Functional Calculations of Molecular Properties
A. Goursot, I. Pápai, and C. A. Daul 799

Density Functional Theory for Jahn–Teller Systems
N. Sukumar 809

Direct Minimization of the Energy in Density Functional Theory
P. Fantucci and S. Polezzo 817

The Dependence of 10Dq upon the Metal–Ligand Distance, *R*, for Transition-Metal Complexes. What is Its Microscopic Origin?
M. Moreno, M. T. Barriuso, and J. A. Aramburu 829

Predictive Chemical Kinetics: Density Functional and Hartree–Fock Calculations on Free-Radical Reaction Transition States
W. H. Green 837

Coulomb-Hole–Hartree–Fock Functional
E. Clementi and D. W. M. Hofman 849

Density Functional Theory Applied to the Excited States of Coordination Compounds
C. Daul 867

The Effects of Nonlocal Gradient Corrections in Density Functional Calculations of Hydrocarbon Radical Hyperfine Structures
L. A. Eriksson, V. G. Malkin, O. L. Malkina, and D. R. Salahub 879

Electronic Structure of Paramagnetic Clusters of Transition Metal Ions. 3. Magnetic Properties and Scattered Wave Description of the Electronic Structure of the Hexanuclear Octahedral Cluster $[Fe_6(\mu_3S)_8(PEt_3)_6](BPh_4)_2$
A. Bencini, M. G. Uytterhoeven, and C. Zanchini 903

Ground-State Properties of $Cd_xSn_{1-x}Te$: The Role of *d*-Electrons
G. H. Grosch, B. Freytag, K.-J. Range, and U. Rössler 919

Geometrical and Spectroscopical Characterizations of Some Complex Entities of Aluminum(III) with Fluoride Ions by LDF-Based Calculations
F. Bouyer, G. Picard, and J.-J. Legendre 927

Application of Second-Order Density Functional Methods to the Calculation of the LiFH Potential Energy Surface
C. Suárez, A. Aguado, C. Tablero, and M. Paniagua 935

Symmetry Breaking and Its Influence on the Correlation Energy for CF_4^+ and CF_3^{2+} Ions
J. M. Garcia de la Vega and E. San Fabian 947

Investigations of Hydrogen-Bonded Systems: Local Density Approximation and Gradient Corrections
R. Kaschner and G. Seifert 957

Density Functional Theory: An Effective Theoretical Tool for the Study of σ Radicals
V. Barone, C. Adamo, and N. Russo 963

Bonding of Acetylene to Copper Atom, Dimer, and Trimer
R. Fournier 973

Self-Consistent Calculations of Total Energies and Charge Densities of Solids Without Solving the Band-Structure Problem
P. Cortona and A. V. Monteleone 987

Ionization Potentials of Atoms Calculated with a Nonlocal Exchange and a Local Correlation Functional
N. A. Cordero, O. V. Gritsenko, A. Rubio, L. C. Balbás, and J. A. Alonso 993

Density Functional Treatment of Water–Carbon Dioxide van der Waals Complex
Y. Abashkin, F. Mele, N. Russo, and M. Toscano 1011

On the Electronic Structure of MoO: Spin-Polarized Density Functional Calculations of Spectroscopic Properties of Low-Lying Quintet, Triplet, and Septet States
E. Broclawik and D. R. Salahub 1017

Applicability to Atoms of a Large Set of Correlation Energy Functionals
E. San Fabián, F. Moscardó, and J. M. Pérez-Jordá 1027

A Density Functional Study of Pseudotetrahedral Metal–Nitrosyl Complexes
F. Bohr, H. Chermette, and M. F. Ruiz-López 1039

An Insight into Optical and EPR Properties of $AgCl_6^{4-}$ and AgF_6^{4-} Complexes Through MS-X(α) and SCCEH Calculations
R. Valiente, J. A. Aramburu, M. T. Barriuso, and M. Moreno 1051

The Chemisorption of Hydrogen on Cu(111): A Dynamical Study
A. Forni, G. Wiesenekker, E. J. Baerends, and G. F. Tantardini 1067

Systematic LSD Investigations on Cationic Boron Clusters: B_n^+ ($n = 2-14$)
I. Boustani 1081

First Principles Calculation of the Optical Properties and Stability of Hydrogenated Silicon Clusters
M. Hirao and T. Uda 1113

List of Participants 1121

Diskette Submission Instructions I

Issue No. 5, 1994

Theoretical and Computational Developments

Natural Polyelectron Population Analysis
R. M. Parrondo, P. Karafiloglou, and E. S. Marcos 1127

Properties, Dynamics, and Electronic Structure of Atoms and Molecules

Evaluation of Cross Sections for X-ray and High-Energy Electron Scattering from Molecular Systems
J. Wang and V. H. Smith, Jr. 1145

Quantum Mechanical Valence Study of a Bond-Breaking–Bond-Forming Process in Triatomic Systems
R. F. Nalewajski, S. J. Formosinho, A. J. C. Varandas, and J. Mrozek 1153

Properties, Dynamics, and Electronic Structure of Condensed Systems

Quantum Chemical Simulations of Hole Self-Trapping in Semi-Ionic Crystals
L. Kantorovich, A. Stashans, E. Kotomin, and P. W. M. Jacobs 1177

Improved Tight-Binding Method
V. A. Telezhkin and A. A. Rafalovich 1199

Two Types of Kramers Rate Equations for Reactions in Condensed Media
S. G. Christov 1219

Molecular Structure, Dynamics, and Function of Biological Systems

The Coordination Chemistry of the Catalytic Zinc Ion in Alcohol Dehydrogenase Studied by Ab Initio Quantum Chemical Calculations
U. Ryde 1229

Announcement 1245

Announcement 1247

Diskette Submission Instructions I

Issue No. 6, 1994

Theoretical and Computational Developments

Fast and Stable Algorithm for the Analytical Computation of Two-Center Coulomb and Overlap Integrals over Slater-Type Orbitals
W. Hierse and P. M. Oppeneer 1249

Lower and Upper Bounds of the Energy Spectrum for Potentials with Multiminima
P. Žitňan 1267

Extrapolation of Real-Space Quantum Chemical Calculations from Finite-Size Super Cells to the Ideal Infinite System. I. Theory
V. Nolting and W. S. Verwoerd 1273

Extrapolation of Real-Space Quantum Chemical Calculations from Finite-Size Super Cells to the Ideal Infinite System. II. Application to One-Dimensional Polymers
V. Nolting and W. S. Verwoerd 1287

On a Generalized Kepler–Coulomb System: Interbasis Expansions
M. Kibler, L. G. Mardoyan, and G. S. Pogosyan 1301

Properties, Dynamics, and Electronic Structure of Atoms and Molecules

Role of Tunneling of Hydrogen in Photoenolization of a Ketone
D. Sengupta and A. K. Chandra 1317

Spectroscopic Properties and Potential Energy Curves of Some Low-Lying Electronic States of AlO, AlO^+, LaO, and LaO^+: An Ab Initio CASSCF Study
A. Márquez, M. J. Capitán, J. A. Odriozola, and J. Fernández Sanz 1329

X-Ray Scattering by Water Molecules Studied by Using Synchrotron Radiation
H. Takeuchi, M. Nakagawa, T. Saito, T. Egawa, K. Tanaka, S. Konaka, and T. Mitsuhashi 1339

A Semiclassical Density Functional Evaluation of the Smoothly Varying Part of the Hartree–Fock Binding Energy in Atoms
Ya. I. Delchev, R. L. Pavlov, K. A. Pavlova, L. P. Marinova, and J. Maruani .. 1349

Erratum

Construction of Linearly Independent Relativistic Symmetry Orbitals for Finite Double-Point Groups Including Time Reversal Symmetry
J. Meyer 1369

Volume Title Page 1373

Subject Index to Volumes 51 and 52 1375

Volume Contents 1381

Author Index to Volumes 51 and 52 1397

Diskette Submission Instructions I